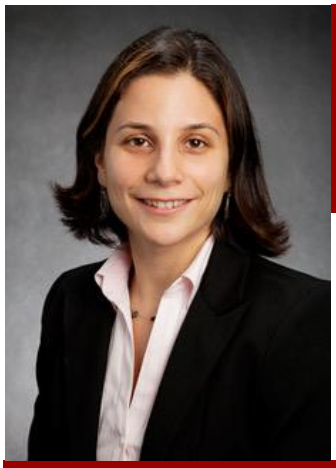

Disorder Effects on Vibrational Transport in Energy Materials

Date : Tuesday, February 19, 2019

Time : 1:00 pm – 2:00pm

Location : Engineering A-131

Professor Elif Ertekin

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University of Illinois, Urbana-Champaign, IL

Abstract:

Disorder in the atomic configuration of a material refers to a lack of regular patterns or predictability in the atomic positions. If the degree of randomness is sufficiently large, one consequence of disorder is localization, which refers to the absence of waves in a disordered medium. The breakdown of the wave picture and the resulting localization of the modes can have strong effects on the electronic, thermal, magnetic, and other properties of materials. In this presentation, I will show some examples from our recent work illustrating the effects of different types of disorder on vibrational transport in energy materials. I will show how established and emerging computational tools can be used to understand the physics that emerges as disorder is introduced. Examples include: the effects of disorder in low-dimensional carbon based materials, hybrid-ordered disordered metamaterials formed by ion beam patterning of silicon, hybrid perovskites which exhibit a dynamic correlated disorder, and diamond-like semiconductors of interest for thermoelectric applications.

Bio:

Elif Ertekin received her PhD in Materials Science and Engineering at UC Berkeley, and then did post-doctoral work at both the Berkeley Nanoscience and Nanotechnology Institute and the Massachusetts Institute of Technology. She is currently an Associate Professor in the Department of Mechanical Science and Engineering at the University of Illinois at Urbana-Champaign, and a Fellow of the National Center for Supercomputing Applications. Her research interests are centered on the use of computational methods spanning from atomistic first principles to continuum mechanics to describe, predict, and better understand material properties, structure/property relations, and phase transformations.